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# Gigatonne One

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## EERE-BETO

## Pitch:

- BECCS—CCS with biofuels, biopower, biomaterials—is key for clean energy-industry futures & for BETO.
- Need to understand spatio-temporal evolution of BECCS sources, sinks, & transportation.
- Massive-scale BECCS only happens within larger CCS system (*Gigatonne One*).
- **BECCS FOCUS:** leverage existing CCS data & tools when possible.

## Tasks:

1. Tool to address national-level [BE]CCS futures/scenarios.
2. Ensemble capability for 100s of CCS pathways, 1000s of runs.
3. BECCS technology analysis.

## Deliverable

- **ROADMAP:** Multi-path spatio-temporal BECCS strategy.

## Gigatonne One: CCS Roadmap for BECCS

Richard Middleton, EES-16 (Los Alamos National Lab)

## Overview

**Objective:** Multi-scenario **roadmap** for national-scale BECCS (bioenergy with CO<sub>2</sub> capture & storage)—ethanol, biopower, biomaterials (e.g., paper/pulpboard)—based on emerging tools, bioeconomy, & **thousands of simulations**.

**Description of Effort:** Nation-wide CCS infrastructure using **SimCCS** framework (including CO<sub>2</sub> storage through **SCO<sub>2</sub>T**). Build (1) BECCS-only scenarios & (2) BECCS integrated with projected nationwide CCS (i.e., Project **Gigatonne One**).

**LANL Unique Capabilities Leveraged:** Unique, R&D 100 Award physics-based tools: (1) **SimCCS** realistically deploy CCS infrastructure based on economics & engineering, perform 1000s of realizations; (2) **SCO<sub>2</sub>T** physics-based estimation of national-scale storage capacities & costs (critical for BECCS).

## Impact

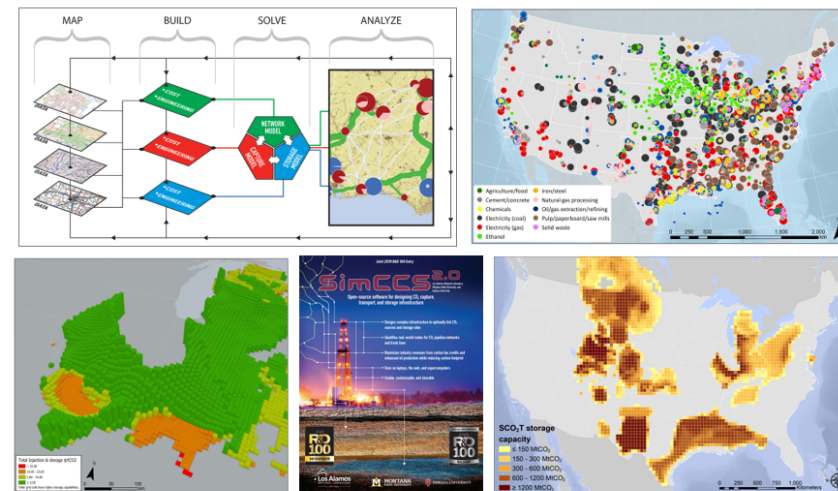
**Benefits:** Key innovation leaps: (1) Multiple scenarios (1000s) based on policy, economics, LCA, & uncertainty; (2) integrated CO<sub>2</sub>-bioeconomy analysis (biofuels/power/materials); (3) driven by realistic CO<sub>2</sub> storage (only at LANL); (4) integrated with emerging CO<sub>2</sub>-based economy; (5) emerging machine-learning. **SimCCS/SCO<sub>2</sub>T** already industry leaders.

## Challenges:

- Scale-up in domain size, solution times, & ensemble analysis.
- Machine learning to process 1000s of scenarios.
- Developing BETO-related CO<sub>2</sub> emissions & scenarios.

**Maturity of Technology:** Current: TRL 4/5. End : TRL 6. Effort focused on data/scenario evolution & technology development.

## Graphical Abstract and Preliminary Results



## Action Plan and Expected Outcomes

## Major Goals and Milestones by Fiscal Year:

- Enhanced capturable-CO<sub>2</sub> database focused on BETO (Yr 1).
- Capture tech. assessment, biopower projection (Yr 1).
- Enhanced **SCO<sub>2</sub>T** database for BECCS (Yr 2).
- Multi-scenario **SimCCS** framework approach (Yr 2).
- **Major deliverable:** BECCS multi-scenario roadmap (Yr 3).

## Proposed Funding (\$k): \$1050k

- Year 1: \$300k (LANL), \$50k (ORNL).
- Year 2: \$300k (LANL), \$50k (ORNL).
- Year 3: \$300k (LANL), \$50k (ORNL).

## Period of Performance (months): 36 months.

**PI:** Richard Middleton, [rsm@lanl.gov](mailto:rsm@lanl.gov), 505-665-8332

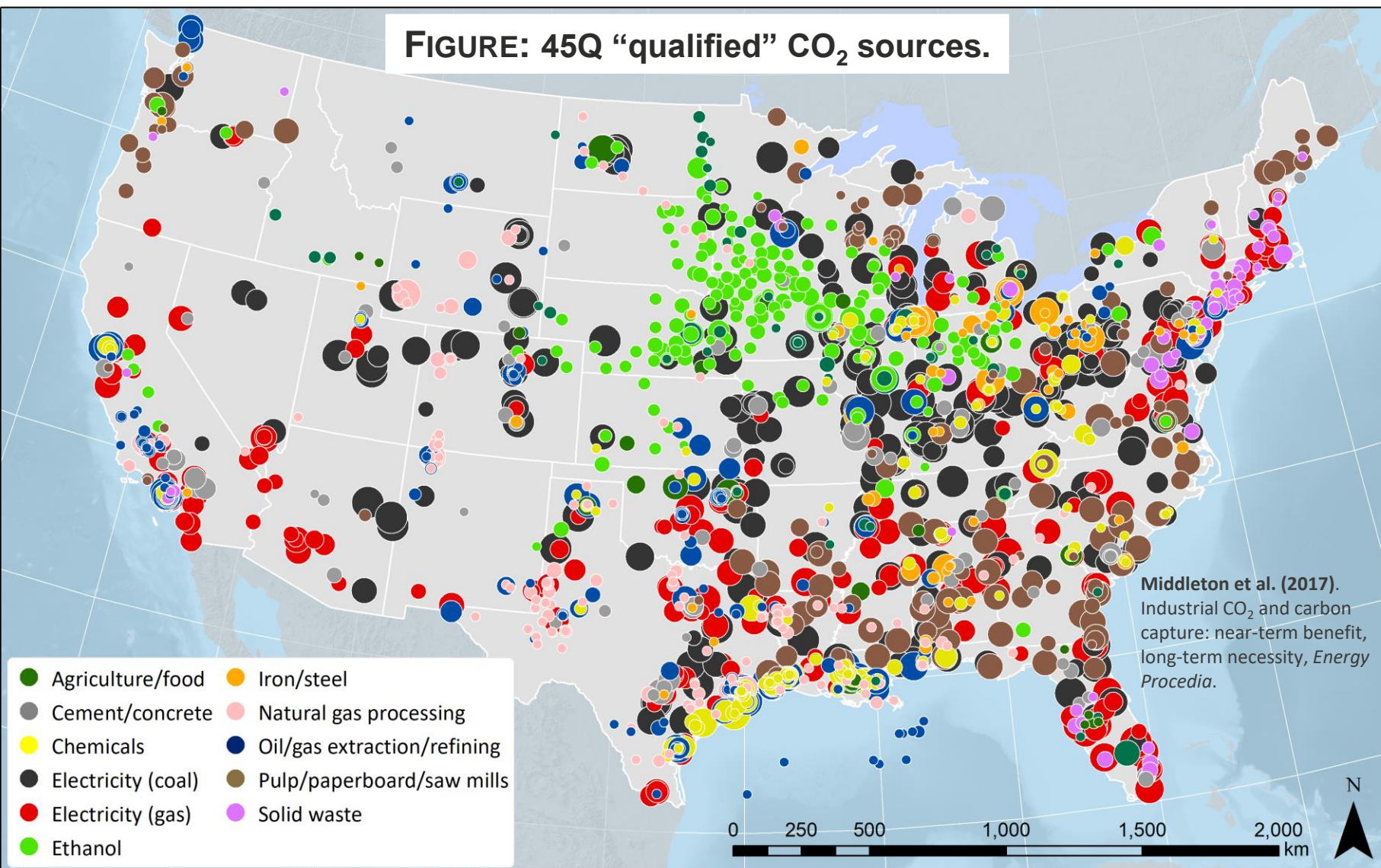
**Making BECCS a National Reality**

Los Alamos National Laboratory



# Background

FIGURE: 45Q “qualified” CO<sub>2</sub> sources.



## Vision

- Gigatonne-scale CCS.
- DOE-FE's CCS vision.

## GIGATONNE ONE:

- Approach to understanding how we get to gigatonne-scale CCS in space & time, including multiple pathways.

## 100s CCS pathways

- **DRIVERS:** CO<sub>2</sub> Incentives, policy, industry targets, oil & CO<sub>2</sub> prices, financing, CCS technologies & economics.



## DOE Investments

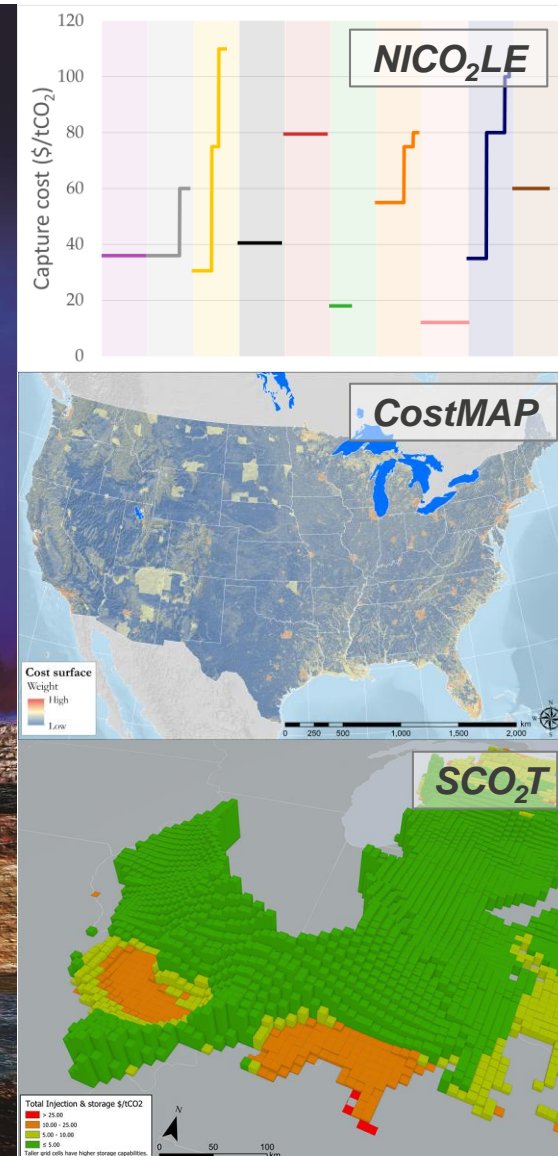
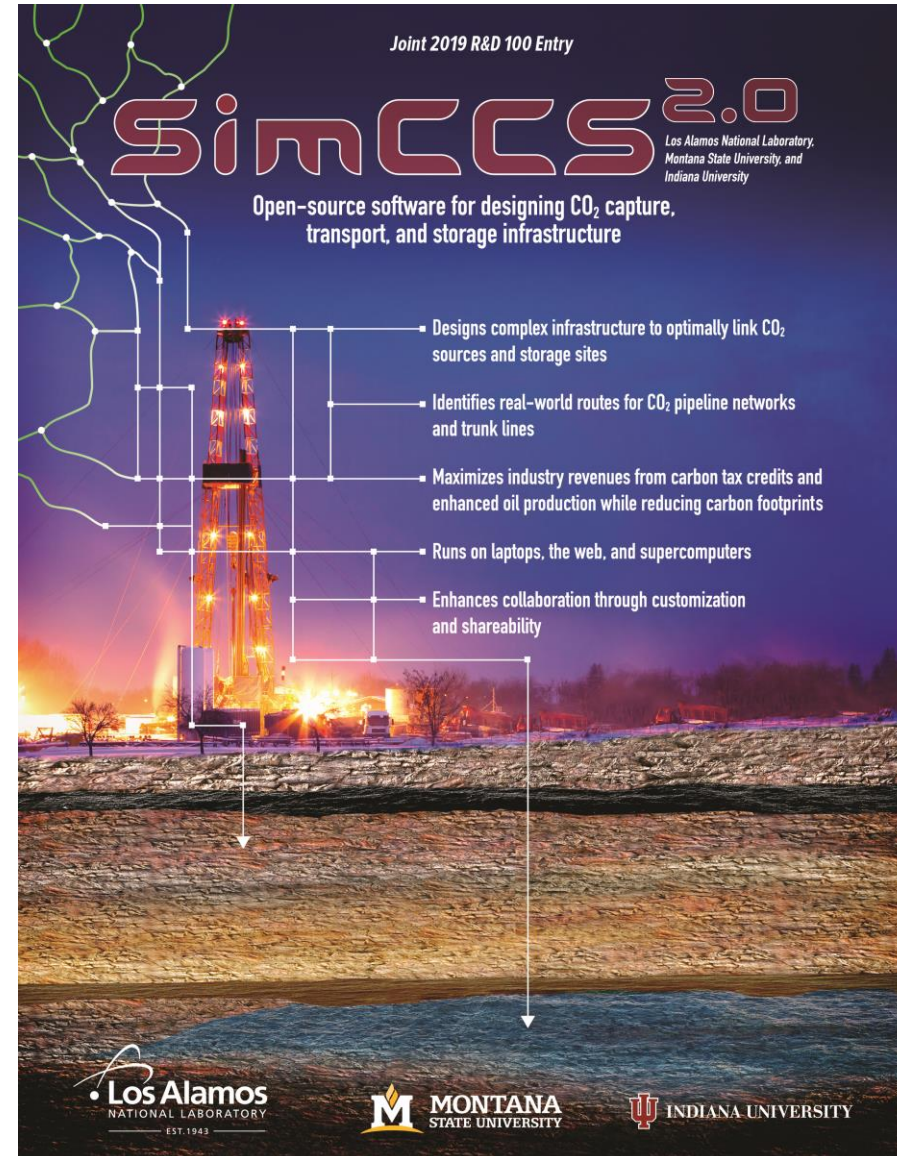
- **SCIENCE, DATA, & TOOLS:** Leverage projects & advances across the CCS value chain.
- **Now:** understand how CCS might unfold.

## SimCCS

- DOE framework for large-scale CCS decisions (advanced source-sink matching).
- Multi-institutional *Team SimCCS*.

## SimCCS tools

1. **SIMCCS:** Framework for integrated source-transport-sink decisions.
2. **SCO<sub>2</sub>T:** Rapid tool that couples physics-based CO<sub>2</sub> injection/storage with economics.
3. **COSTMAP:** Pipeline routing and candidate network generation.
4. **NICO<sub>2</sub>LE:** Capturable-CO<sub>2</sub> database, sources broken down by CO<sub>2</sub> streams & economics.



# Challenges

## Data challenge

- Building national capture, transport, & storage databases.

## Simulation challenge

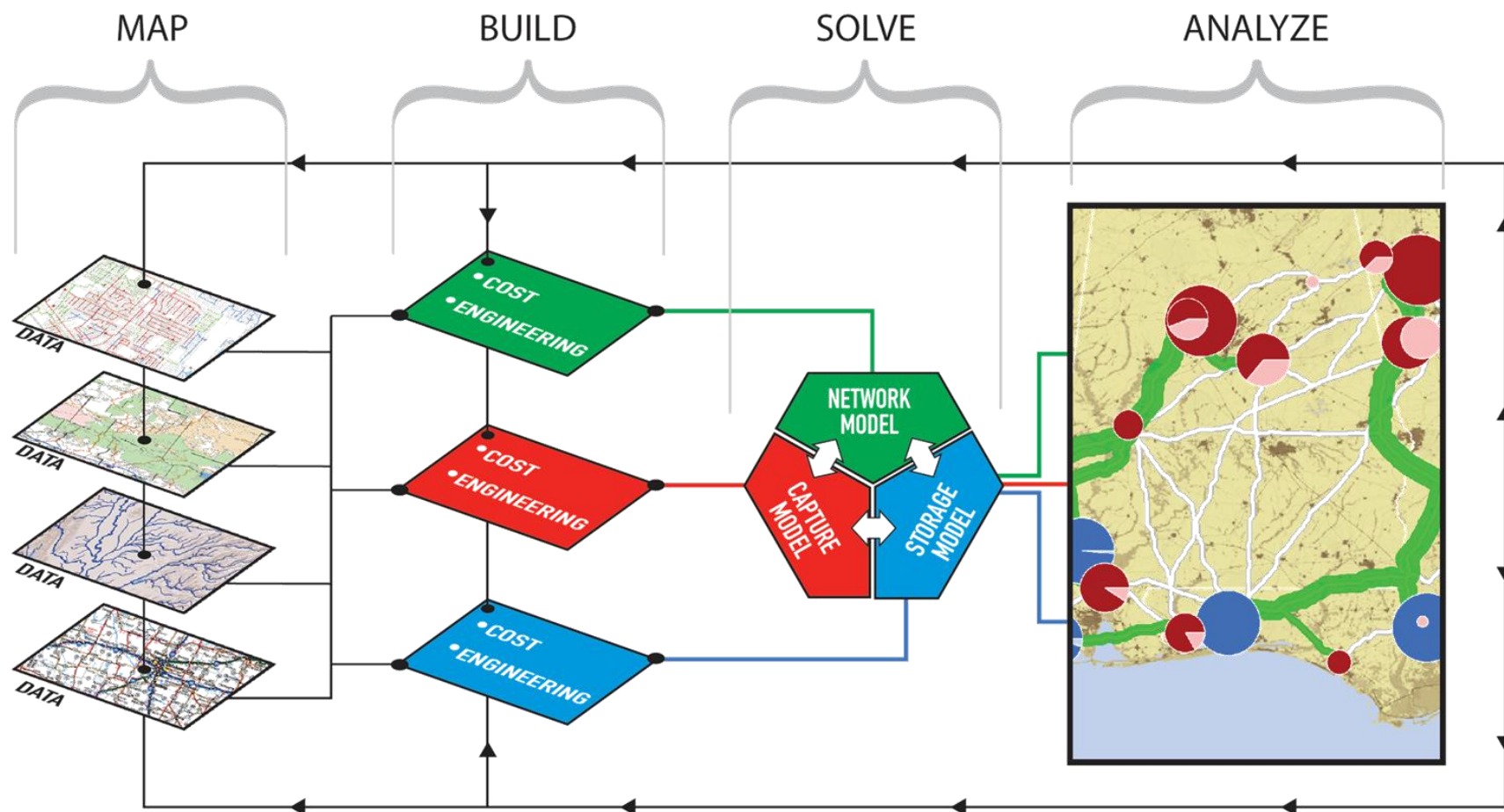
- Realistic national-scale simulations (single run).
- Heuristics, machine learning?

## Ensemble challenge

- Uncertainty + pathways = 1000s realizations.
- Paradigm shift.

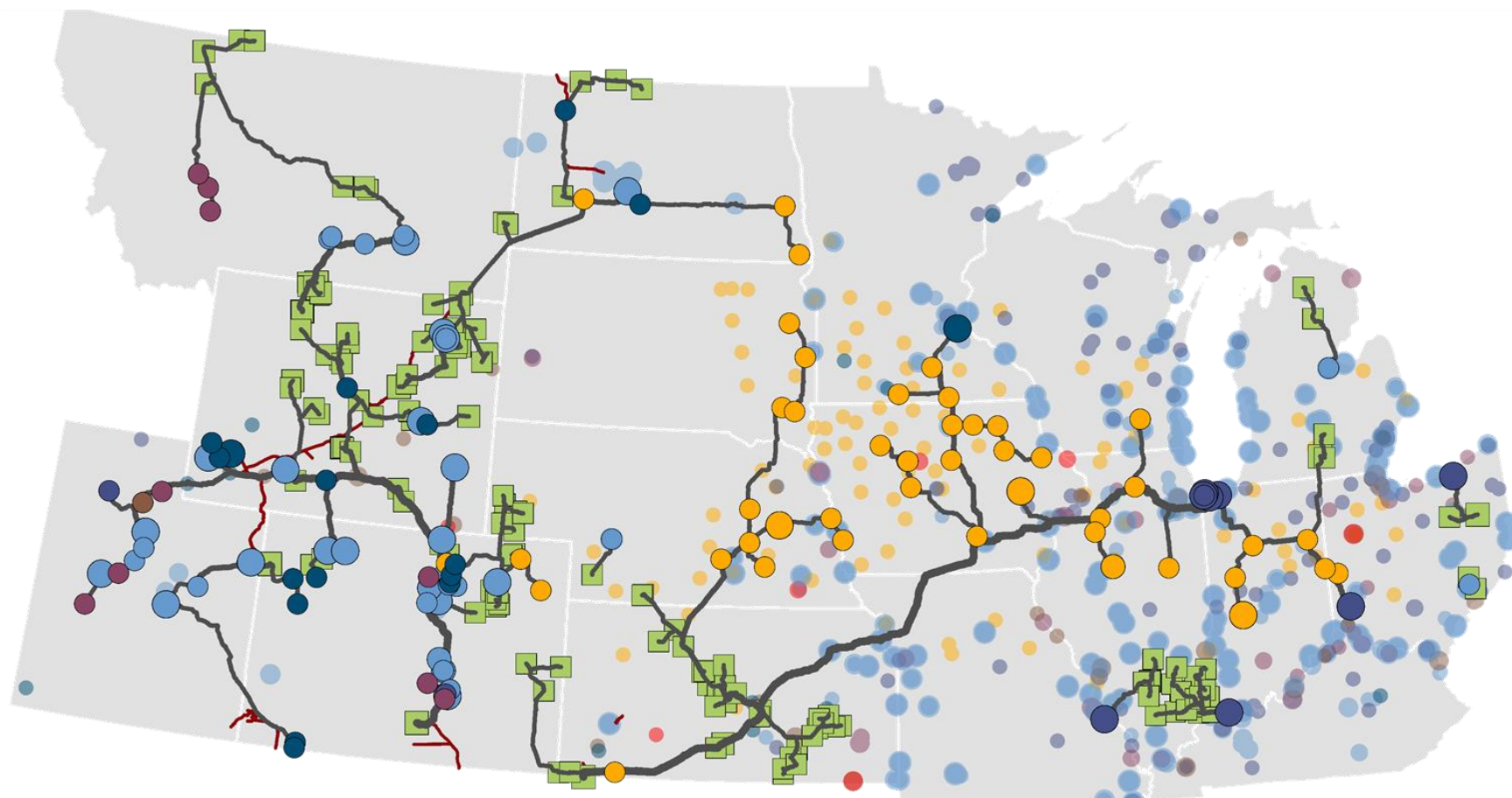
## Analysis challenge

- Machine learning to explore 1000s pathways.





# Scenario Analysis



## Network Infrastructure

### Pipelines & Sinks

Volumetric  
Flow in million  
metric tonnes

Size of Sinks  
in annual million  
metric tonnes

### Top CO2 Sources by Industry & Volume

Petroleum & Natural Gas  
Cement  
Industrial  
Ammonia & Fertilizers  
Ethanol  
Electricity

### Additional CO2 Sources & Sinks

Size of Source  
in annual million  
metric tonnes  
Existing  
Pipeline  
Refineries & Chemicals  
Ammonia  
Electricity  
Industrial  
Cement  
Ethanol  
Petroleum & Natural Gas  
CO2 Sinks (EOR & Saline)

<http://www.betterenergy.org/blog/press-release-14-state-work-group-releases-federal-state-recommendations-carbon-capture/>

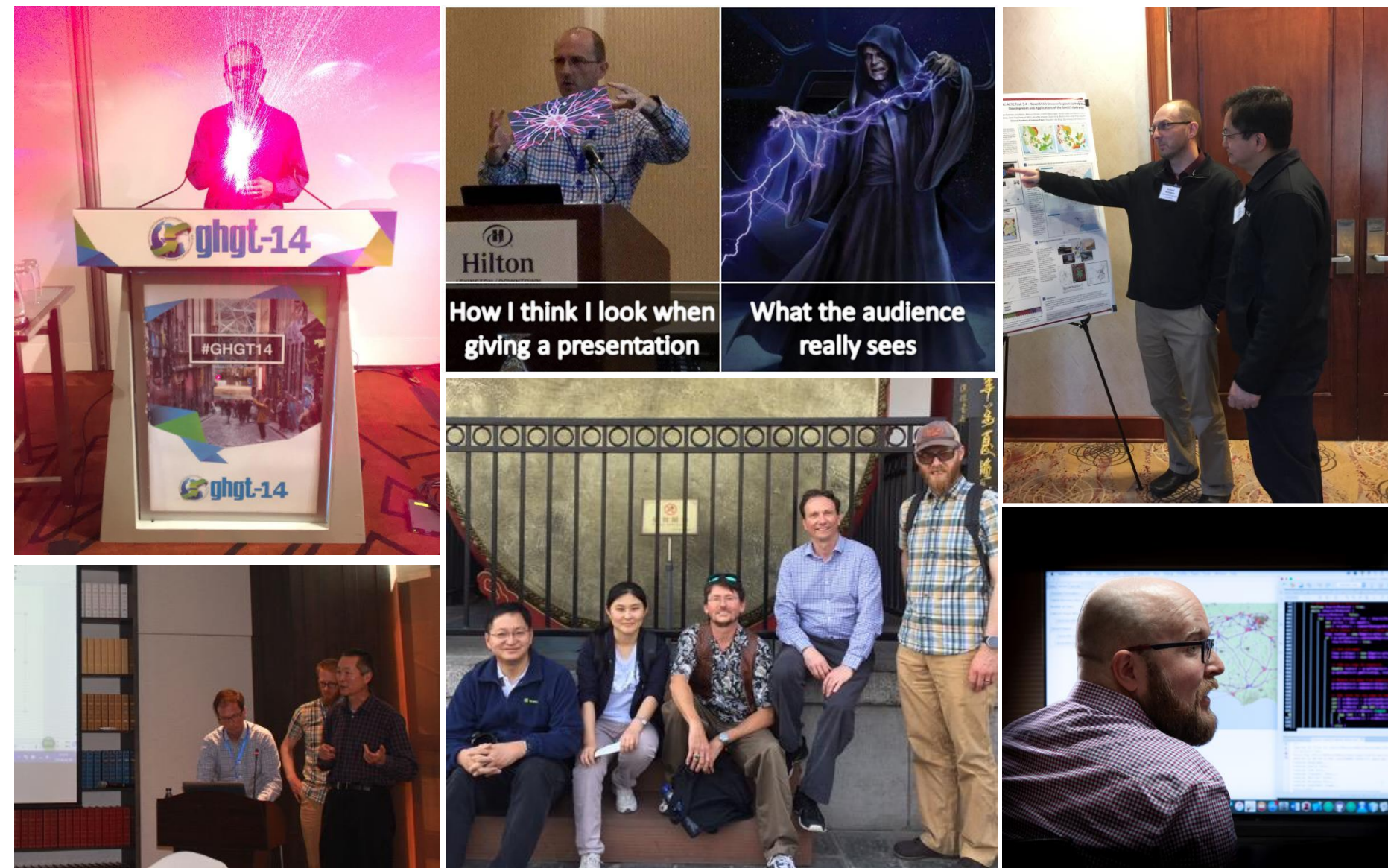
## “What if?” scenarios

- Impact of policy & incentives?
- Marginal return (costs, CO<sub>2</sub> amount) from federal investment in expanding industry-funded trunk lines?
- What does coal-dominated Gigatonne One look like?
- LCA-aware CO<sub>2</sub> incentives?
- Change in CCS spatio-temporal deployment given technology price points?
- Massive CCS storage complexes vs. distributed storage (cost, risk, capacity)?



Additional Slides

# Team SimCCS



## Team

- ~30 participants, 16 institutions.

## Partners

- **UNIVERSITIES:** Arizona, Indiana, Montana, Ohio, California, Utah, Virginia, West Virginia, Wyoming.
- **INSTITUTIONS:** Battelle, Chinese Academy of Sciences, EPRI, Enhanced Oil Recovery Institute, Great Plains Institute, Kansas Geological Survey, NREL.
- **INDUSTRY:** Advanced Resources International, Archer Daniels Midland, BP, Duke Energy, Glenrock Petroleum, Jupiter Oxygen, Occidental Petroleum, Southern Company.

## Scientific visibility

- **PAPERS:** ~30 publications, 1,000+ citations.
- **PEOPLE:** ~100 (published, used, developed, funded).



# Integrated CCS Decisions: *SimCCS*

## Why: CCS drivers

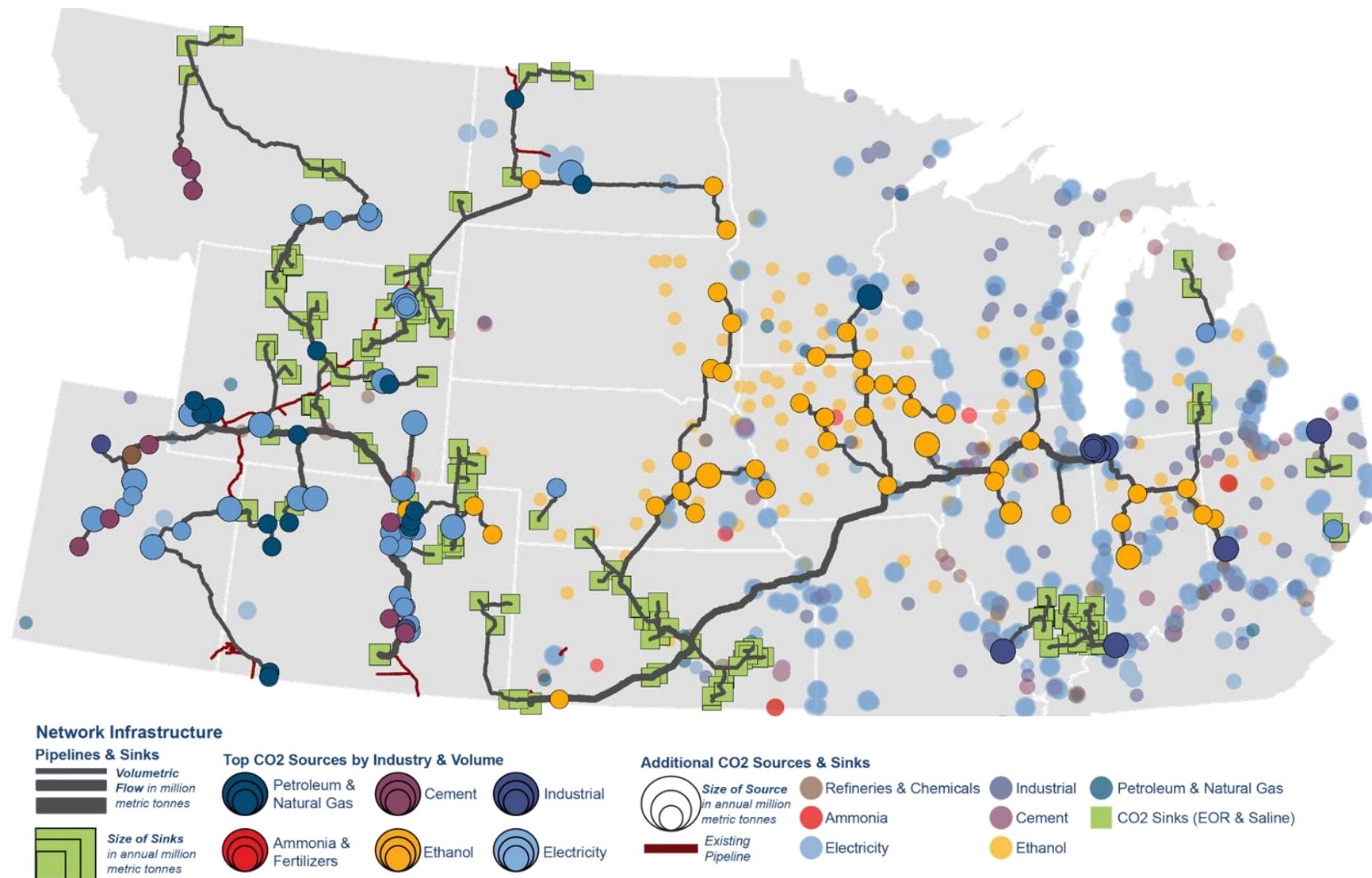
- **GLOBAL:** Climate mitigation.
- **US:** Economic incentives.
- **CHINA:** ETS (CCS in 2030).
- **INDUSTRY:** Carbon footprints.

## How: Decision framework

- CCS Infrastructure design.
- Open-source, Java-based, HPC-enabled framework.

## What: Scientific visibility

- **PAPERS:** 20+ publications, 1,000+ total citations.
- **People:** ~100 (published, used, developed, funded).
- **R&D 100 AWARDS:** *Software & Services and Corporate Social Responsibility* (2019).



# Overview

## SimCCS Framework

- Optimization
- Integrated capture and storage
- Define economic engineering

## CAPTURE

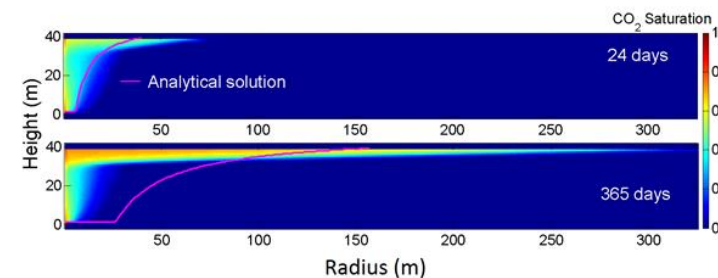
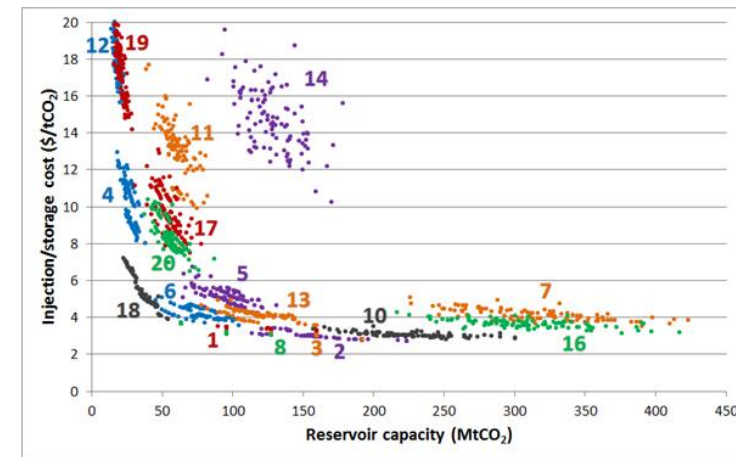
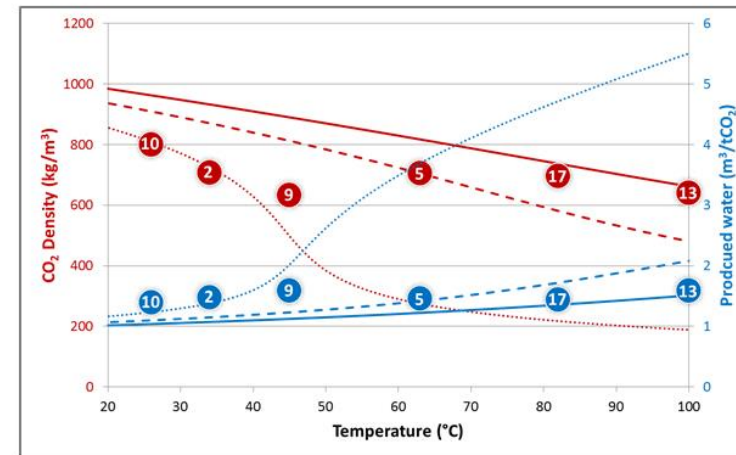
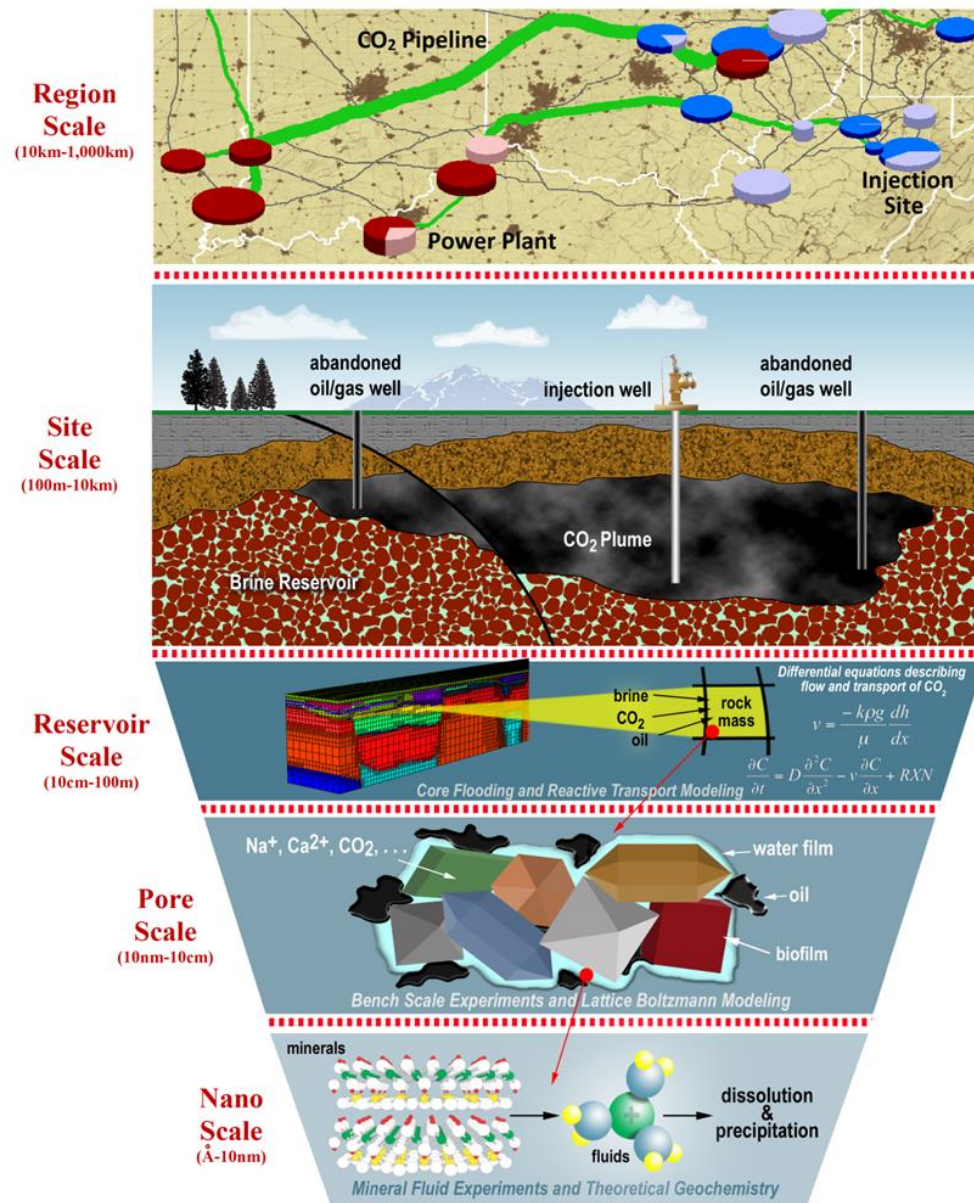
- Literature value
- IECM model

## TRANSPORT

- Cost surface
- Candidate network

## STORAGE

- Reduced or no leakage ( $\text{SCO}_2\text{T}$ )
- Custom cost



RAL

CO<sub>2</sub> cost-  
questeredCCS  
cture

cations

en capture,  
d storage



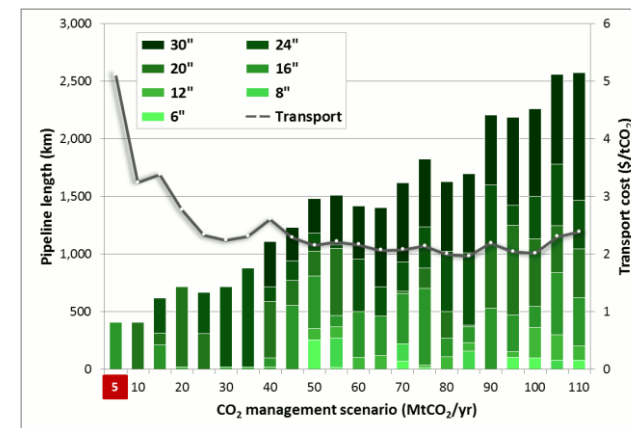
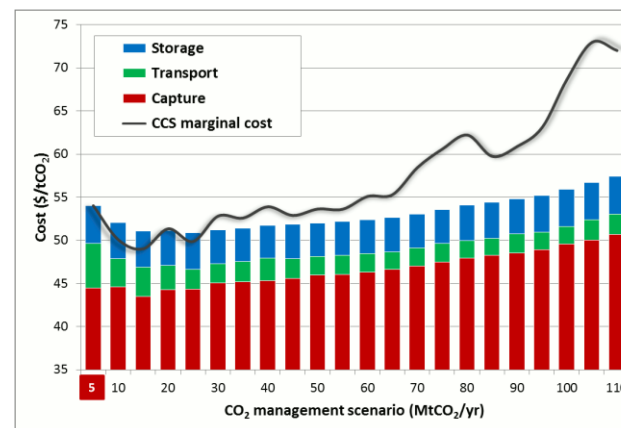
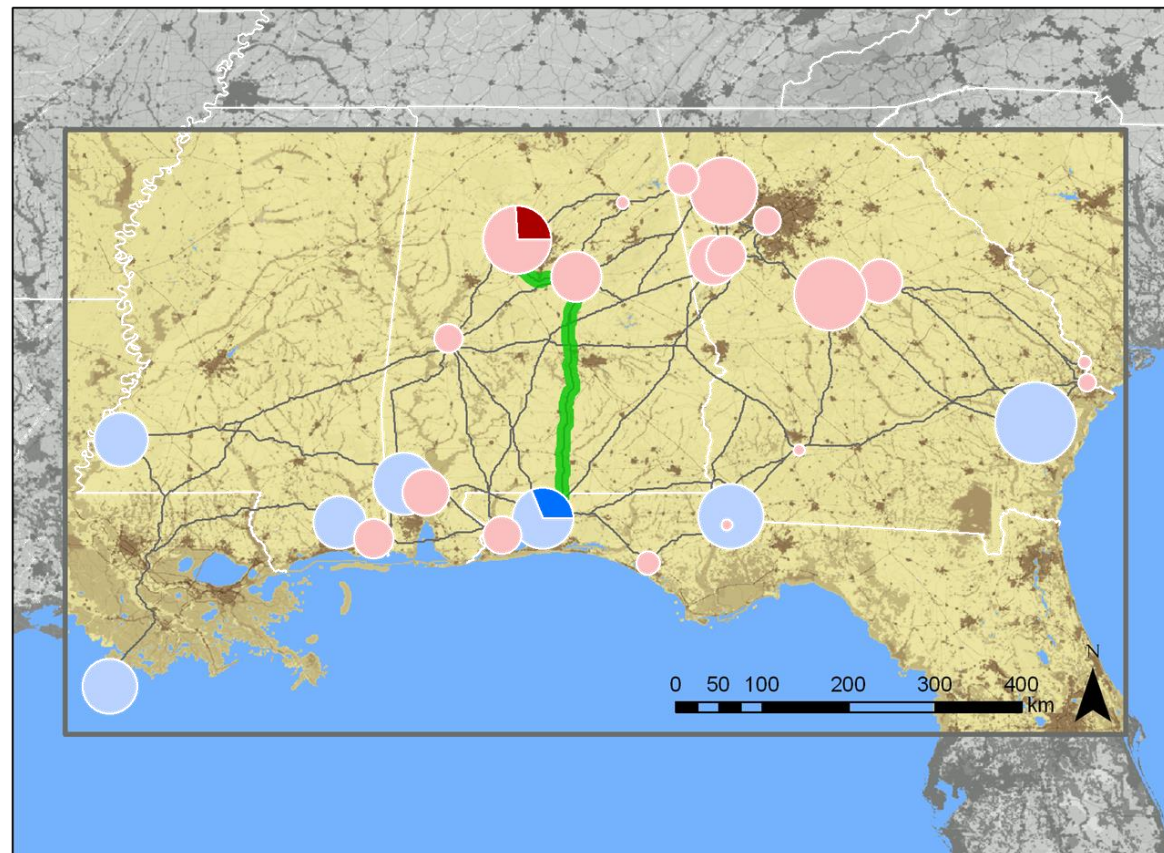
# SimCCS: Analysis

## Approach

- Cap-and-trade version of *SimCCS* → set CO<sub>2</sub> cap (or target) & minimize costs.
- Inverse: set economic cap and maximize CO<sub>2</sub>.

## Southern Company

- Ten year business plan and CO<sub>2</sub> emissions strategy.
- 20 coal-fired plants: 156 MtCO<sub>2</sub>/yr emissions.
- 65 individual boilers → boiler level accuracy.
- **CAPTURE COSTS:** \$46-102/tCO<sub>2</sub> (plant) & \$41-166/tCO<sub>2</sub> (boiler).
- **STORAGE:** 3.4 GtCO<sub>2</sub> in 7 sinks, 113 MtCO<sub>2</sub>/yr over 30 years.
- **STORAGE COSTS:** \$3.78-8.60/tCO<sub>2</sub>.



Middleton et al. (2012). The cross-scale science of CO<sub>2</sub> capture and storage: from pore scale to regional scale, *Energy and Environmental Science*, [doi.org/10.1039/c2ee03227a](https://doi.org/10.1039/c2ee03227a).

# Capture

## Jumpstarting CCS

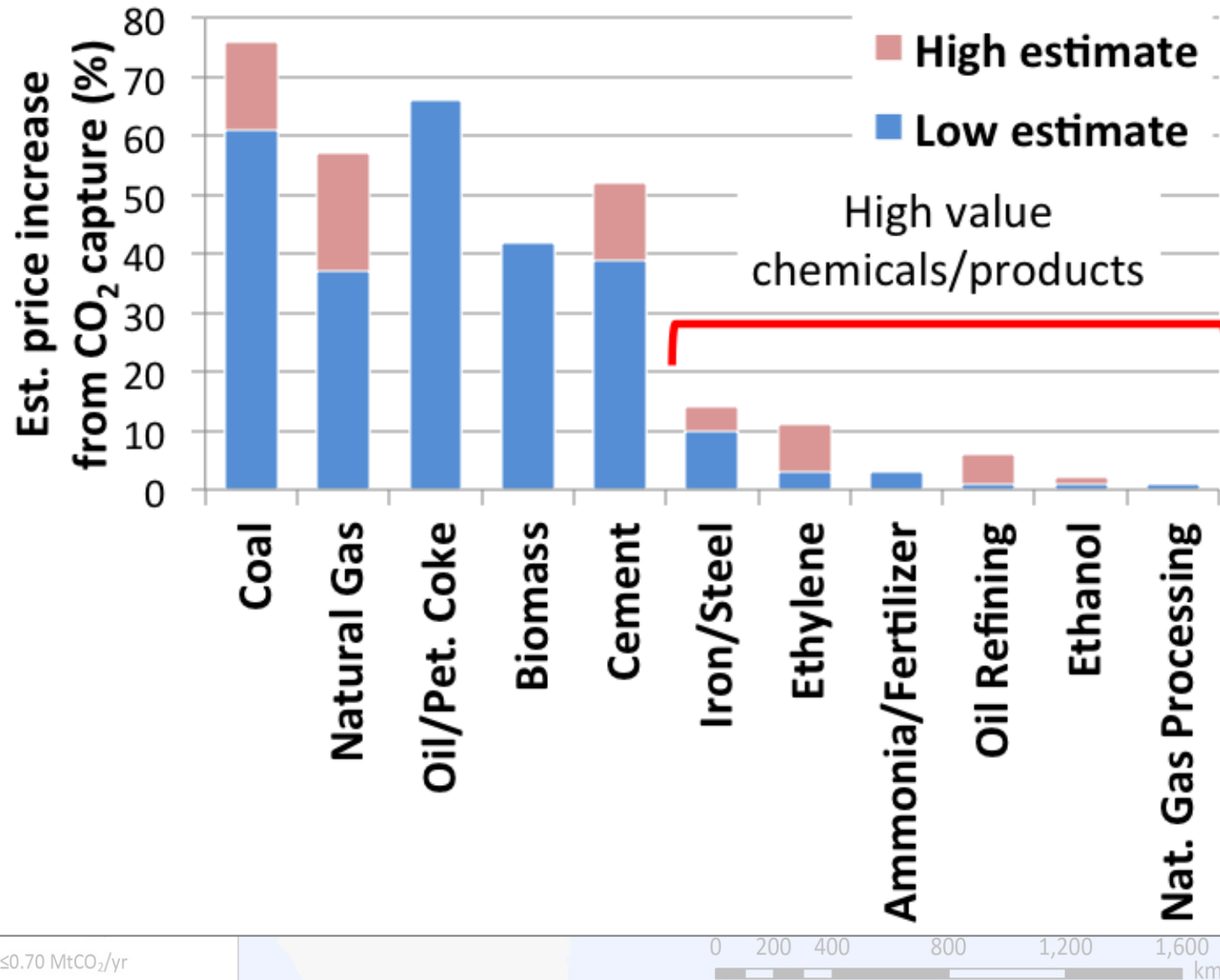
- Developed the concept of high-value chemicals and products (HVCPs).
- HVCPs: CCS opportunities that can be economically absorbed by supply chains.

## Approach

- Life-cycle analysis.
- Infrastructure optimization.
- CCS economics.

## Take home message

- First study to identify new way to use industrial CO<sub>2</sub> to jumpstart CCS.





# Transport

## Routing & networks

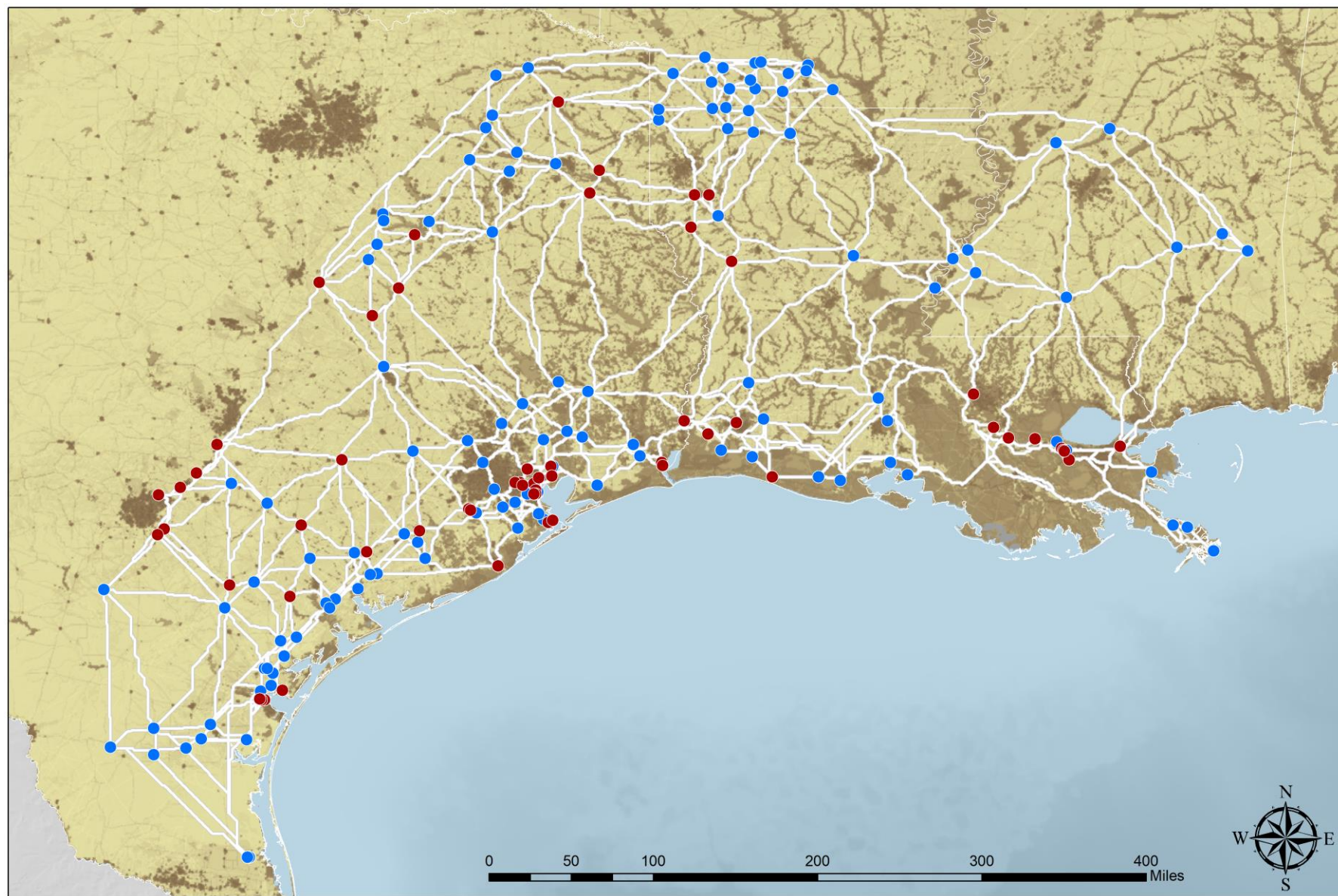
- Most advanced weighted cost surface for pipeline routing.
- Unique approach for converting raster data to vector network.

## Approach

- Optimization.
- GIScience.
- Decision analysis.

## Take home message

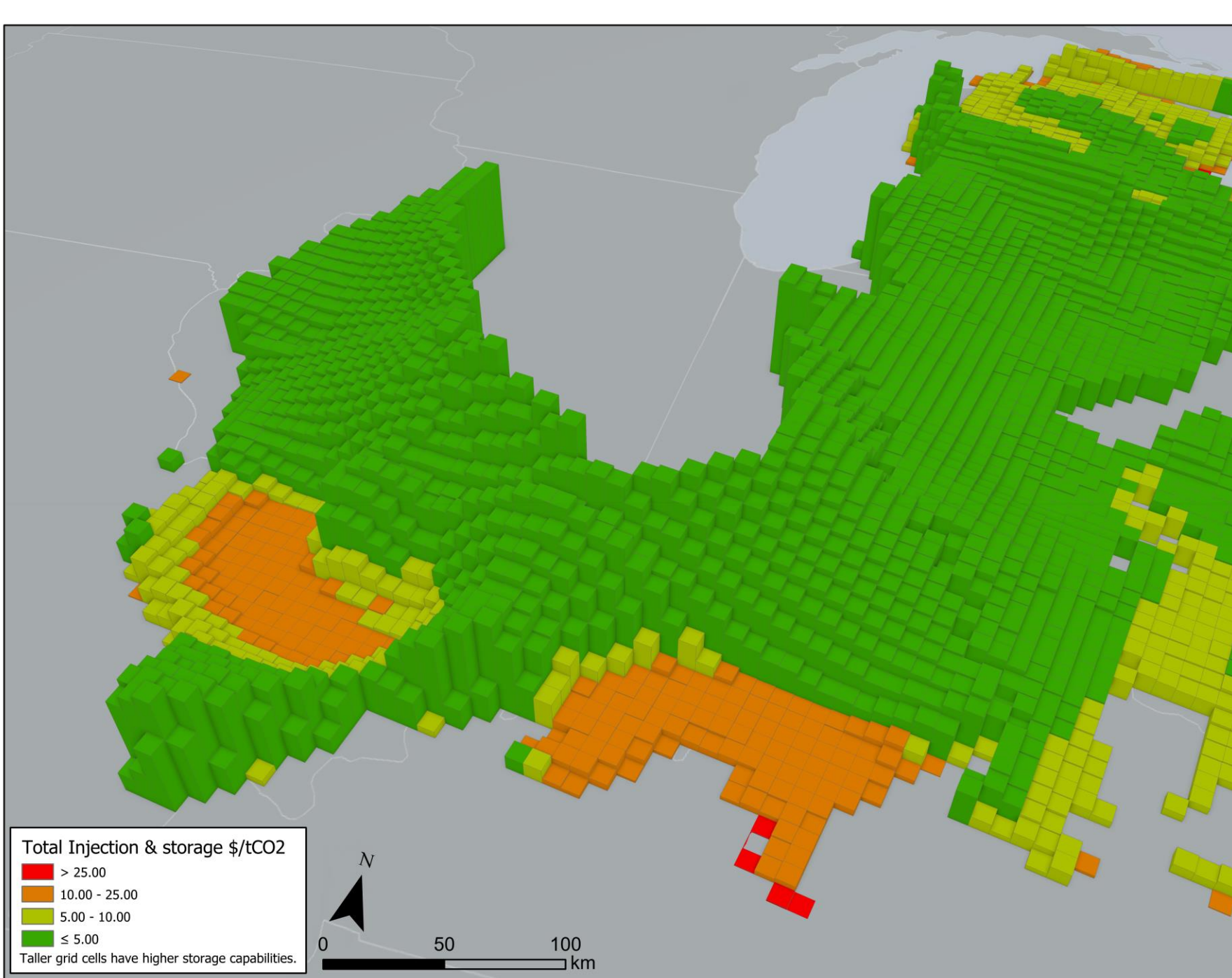
- Transformed pipeline routing and developing potential pipeline networks.



Middleton et al. (2012). Generating candidate networks for optimization: the CO<sub>2</sub> capture and storage optimization problem, *Computers, Environment, and Urban Systems*, [doi.org/10.1016/j.compenvurbsys.2011.08.002](https://doi.org/10.1016/j.compenvurbsys.2011.08.002).

Hoover, Yaw, Middleton et al. (2019). CostMAP: An open-source software package for developing cost surfaces, *International Journal of Geographical Information Science*, [doi.org/10.1080/13658816.2019.1675885](https://doi.org/10.1080/13658816.2019.1675885).





## APPROACH

# Storage: $\text{SCO}_2\text{T}$

## What?

- New tool being developed by *Team SimCCS*.
- New database leveraging NATCARB & USGS.

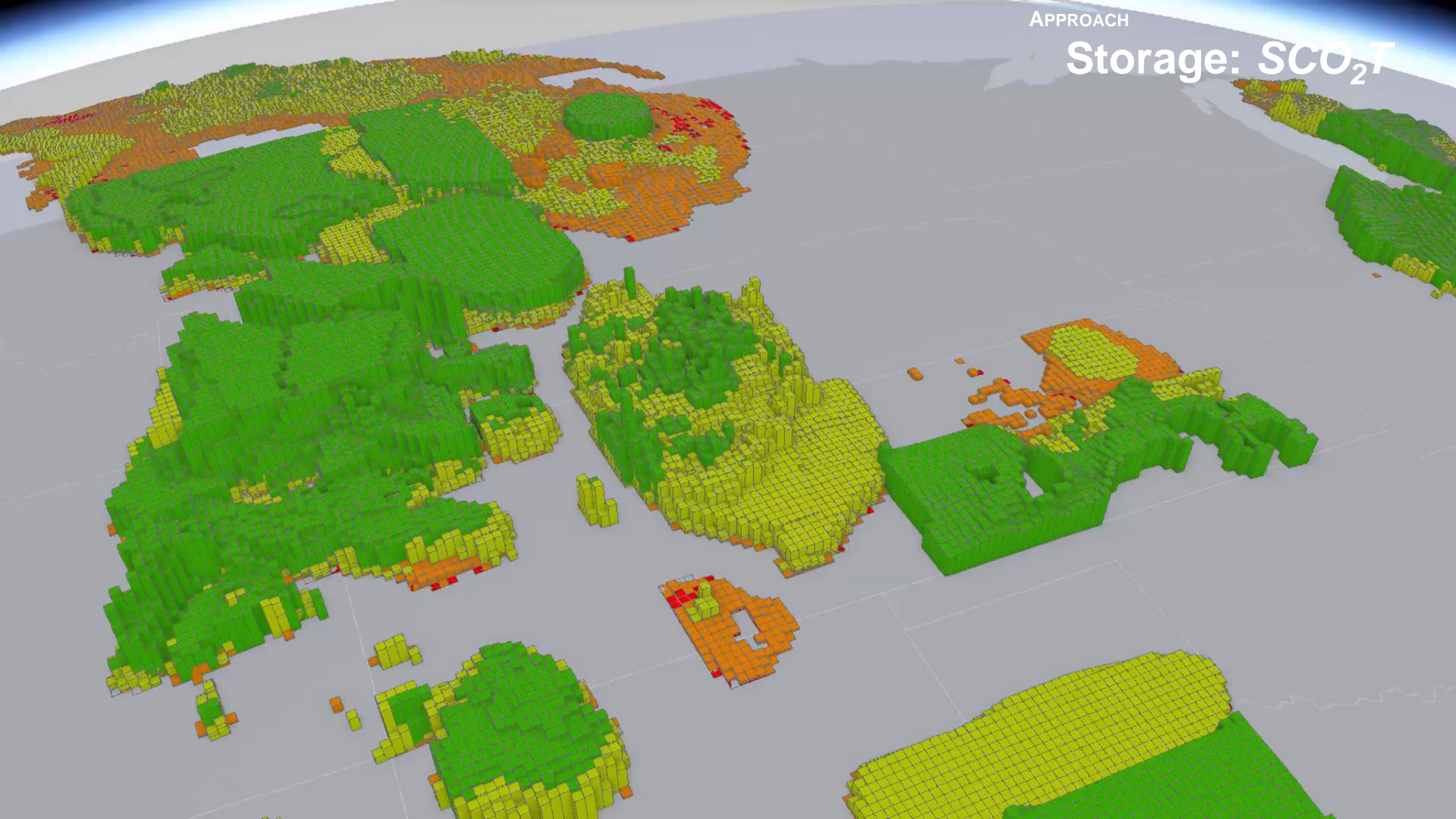
## Unique capability

- Realistic simulated injection (not volumetric analysis).
- Coupled sequestration engineering & economics.
- Replicable & uncertainty.
- Operational tool (e.g., well spacing, 1 MtCO<sub>2</sub>/yr).
- Impact of brine treatment.
- Nationwide understanding of CO<sub>2</sub> sequestration.



APPROACH

Storage:  $\text{SCO}_2T$



## Goal

- Represent complex physics in a reduced model.

## Approach

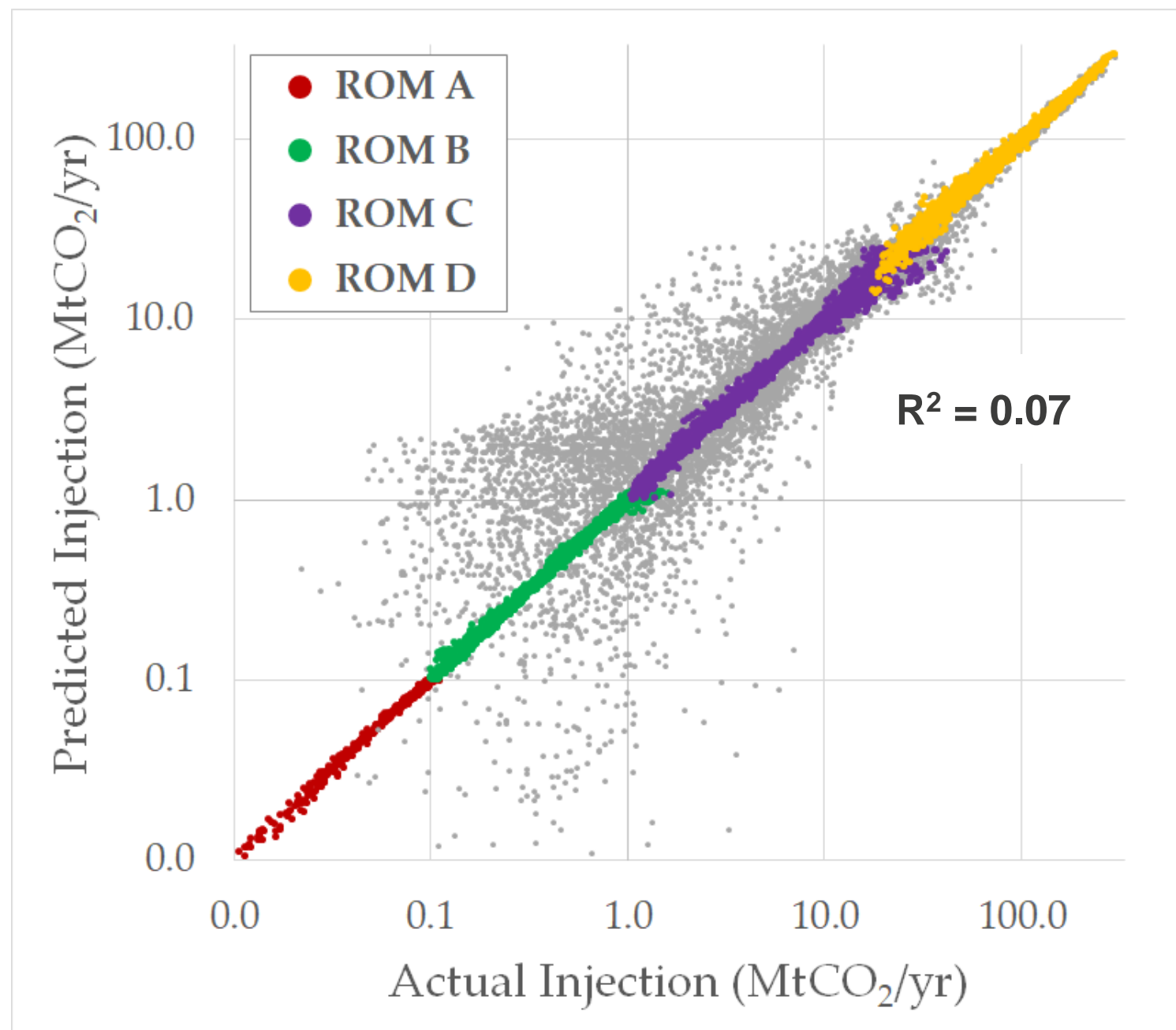
- Use complex, fully-physics simulators to train reduced models: <https://fehm.lanl.gov/>.

## Approach

- 10,000 FEHM runs, ~3 weeks on ~64 cores.
- Vary depth, thickness, permeability, porosity, temperature.
- Train multiple ROMs.

## Take home message

- Transformational approach to capturing complex physics in rapid-running ROM.



Chen, ..., Middleton (2020). Frankenstein's ROMster: Avoiding pitfalls of reduced-order model development, *International Journal of Greenhouse Gas Control*, [doi.org/10.1016/j.ijggc.2019.102892](https://doi.org/10.1016/j.ijggc.2019.102892).



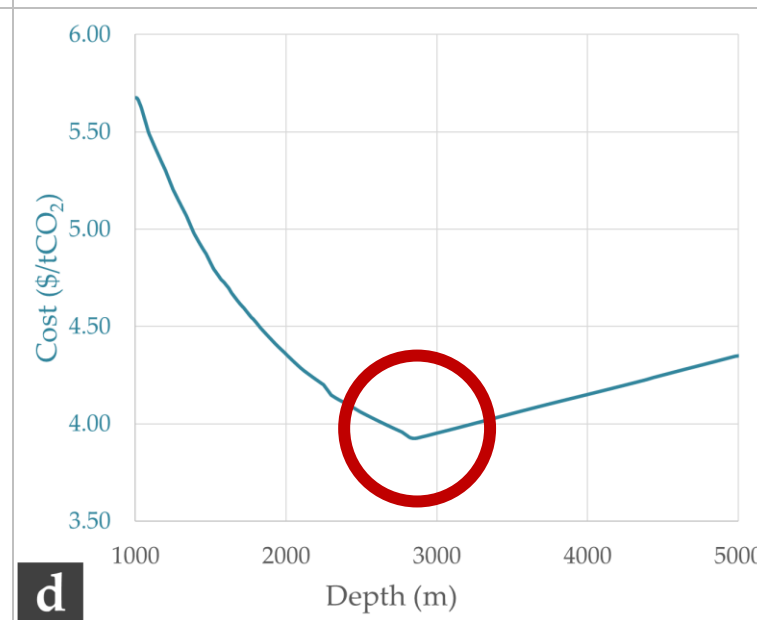
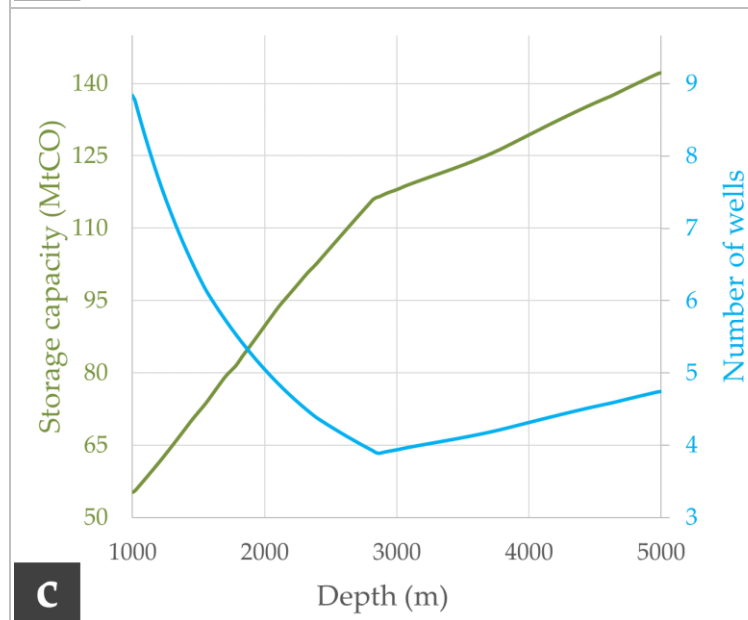
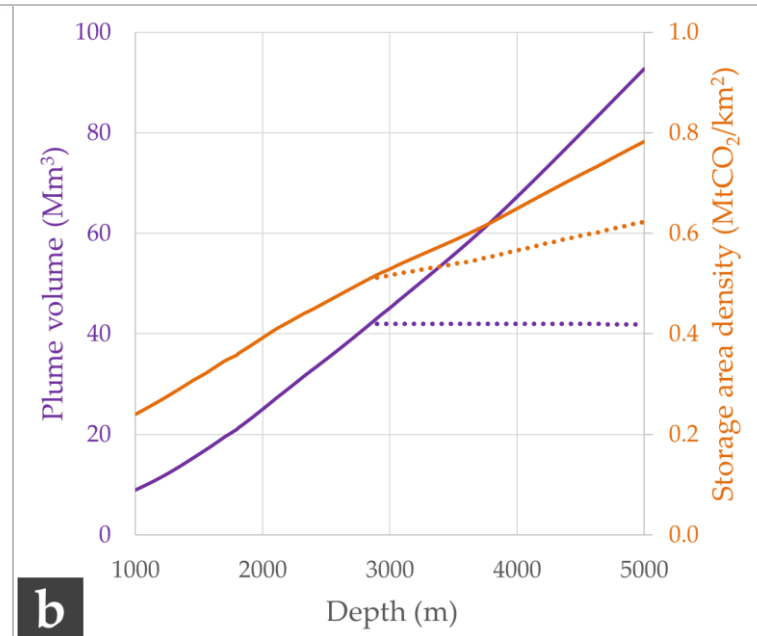
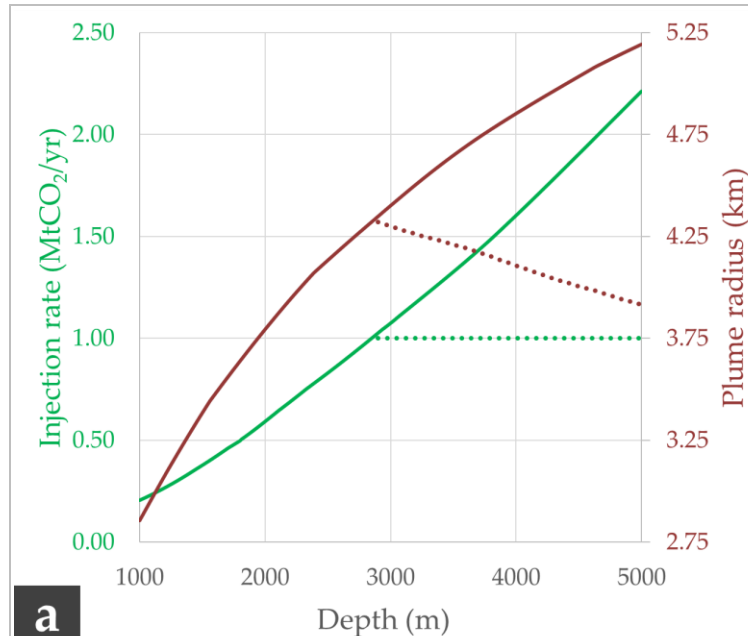
# SCO<sub>2</sub>T

## Sequestration science

- Build ROMster approach into standalone tool.
- Rapidly assess impact of geology on CO<sub>2</sub> injection, plume characteristics, and storage capacity.
- Depth: can increase and decrease sequestration costs.

## Take home message

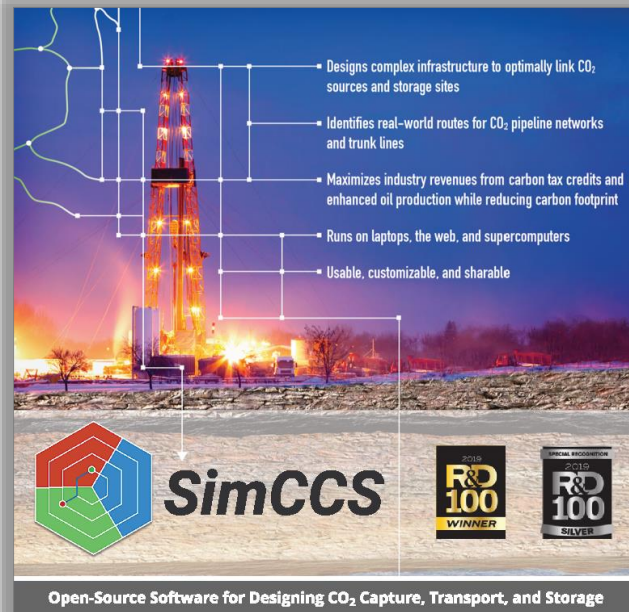
- New & innovative understanding of sequestration science.



Middleton et al. (2020). Great SCO<sub>2</sub>T! Rapid carbon sequestration science and screening, *Applied Energy* (In Review).

Middleton et al. (2020). Beam me up SCO<sub>2</sub>T: identifying geologic characteristics and operational decisions to meet global carbon sequestration goals, *Energy and Environmental Science* (In Review).

# Flyers: *SimCCS* and *SCO<sub>2</sub>T*



- Designs complex infrastructure to optimally link CO<sub>2</sub> sources and storage sites
- Identifies real-world routes for CO<sub>2</sub> pipeline networks and trunk lines
- Maximizes industry revenues from carbon tax credits and enhanced oil production while reducing carbon footprint
- Runs on laptops, the web, and supercomputers
- Usable, customizable, and sharable

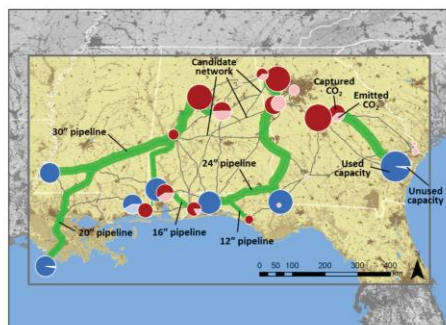
**SimCCS**

2018 R&D 100 WINNER  
2019 R&D 100 SILVER

Open-Source Software for Designing CO<sub>2</sub> Capture, Transport, and Storage

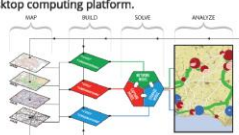
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simccs.com

**SimCCS**

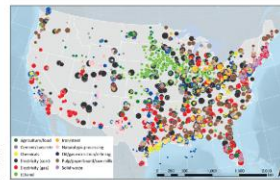


**Figure:** *SimCCS* infrastructure design for southeast United States case study with a target capture amount of 110MtCO<sub>2</sub>/yr over a 30-year project life. The data for this case study is included in the *SimCCS* software repository.

**About *SimCCS*:** Introduced in 2009, *SimCCS* is an optimization model for integrated system design that enables researchers, stakeholders, and policy makers to design carbon, capture, and storage (CCS) infrastructure networks. In the past two years, *SimCCS* was completely redesigned and is now a portable software package, useable and shareable by the CCS research, industrial, policy, and public communities. *SimCCS* integrates multiple new capabilities including a refined optimization model, novel candidate network generation techniques, and optional integration with high-performance computing platforms. Accessing user-provided CO<sub>2</sub> source, sink, and transportation data, *SimCCS* creates candidate transportation routes and formalizes an optimization problem that determines the most cost-effective CCS system design. This optimization problem is then solved either through a high-performance computing interface, or through third-party software on a local desktop computing platform.



**Figure:** *SimCCS* end-to-end workflow (left to right). The MAP tool provides data from a geodata service and enables selection of an area of sources and sinks for which a candidate pipeline network will be designed. The BUILD tool generates *SimCCS* problems based on the costs and engineering requirements of CO<sub>2</sub> capture (red), transport (green), and storage (blue) for the area selected by MAP. The SOLVE tool (red-blue-green hexagon) generates a candidate pipeline network. The ANALYZE tool allows users to consider the candidate network. New candidates can be generated with the different weights being given to various decision-making factors. The arrows encircling the figure represent the workflow's iterative nature: the entire process can be repeated as often as needed.



**Figure:** Major U.S. industrial sources of CO<sub>2</sub> (data source: Middleton et al. [2014], "CO<sub>2</sub> Deserts: Implications of Existing CO<sub>2</sub> Supply Limitations for Carbon Management," *Environmental Science & Technology* 48, 11713–11720).

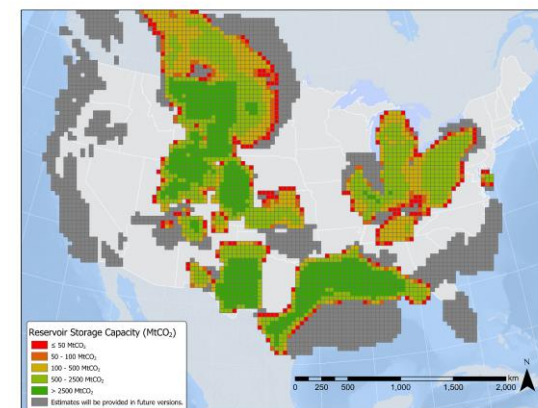


## *SCO<sub>2</sub>T*: An open-source tool for CO<sub>2</sub> storage estimates.

- First nationwide understanding of CO<sub>2</sub> injection rates, storage capacities, and cost.
- Links sequestration engineering to economics.
- Realistic storage estimates using physics-based CO<sub>2</sub> injection
- Enables new understanding of sequestration science.

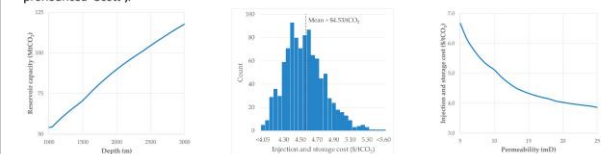
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simccs.com

**SCO<sub>2</sub>T**



**Figure:** Reservoir storage capacity estimates for select deep saline formations throughout North America using *SCO<sub>2</sub>T*. Results generated using the *SCO<sub>2</sub>T* Database, an aggregation of sink parameters from studies by the U.S. Department of Energy, U.S. Geological Survey, and the National Energy Technology Laboratory.

**About:** CO<sub>2</sub> capture and storage (CCS) technology is likely to be widely deployed in coming decades in response to major climate and economics drivers: CCS is part of every major climate policy that limits global warming to 2°C and receives significant CO<sub>2</sub> tax credits in the United States. These drivers are likely to stimulate capture, transport, and storage of hundreds of millions or billions of tonnes of CO<sub>2</sub> annually. A key part of the CCS puzzle will be identifying and characterizing suitable storage sites for vast amounts of CO<sub>2</sub>. We introduce a new fast-running, open-source, no-installation-required tool called *SCO<sub>2</sub>T* (Sequestration of CO<sub>2</sub> Tool, pronounced "Scott").



**Figure:** *SCO<sub>2</sub>T* uses sensitivity and uncertainty analyses from reservoir parameters to help industry and policy makers properly understand CCS capabilities in their regions.